

E -restricted double traces

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Abstract

For a graph G and $E \subseteq E(G)$, E -restricted strong trace is a closed walk which traverses every edge from E once in each direction and every other edge twice in the same direction. In addition, every time a strong trace come to a vertex v from $N \subseteq N(v)$ it continues to $u \notin N$, for $1 \leq |N| < d(v)$. We characterize graphs admitting E -restricted strong traces and explain how this result can be used as an upgrade of mathematical model for self-assembling nanostructure design first presented by Gradišar et al. in [Design of a single-chain polypeptide tetrahedron assembled from coiled-coil segments, Nature Chemical Biology 9 (2013) 362–366].

Keywords: E -restricted strong trace, d -stable trace, spanning tree, self assembling, nanostructure design

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1 Introduction

In 2013 Gradišar et al. in [11] presented a novel self-assembly strategy for polypeptide nanostructure design and also experimentally demonstrated the formation of the tetrahedron that self-assembles from a single polypeptide chain comprising 12 concatenated coiled coil-forming segments separated by flexible peptide hinges. During the construction the path of the polypeptide chain is guided by a defined order of segments that traverse each edge of the polyhedron (tetrahedron in that particular example) exactly twice. Therefore, to serve as an appropriate mathematical description, strong (and d -stable) traces were later introduced in [5], as closed walk which traverses every edge of graph exactly twice and for every vertex v , there is no subset N of its neighbors, with $1 \leq |N| < d(v)$ ($1 \leq |N| \leq d$), such that every time the walk enters v from N , it also exits to a vertex in N . That also represents a generalization of previously used mathematical model from [12] to graphs with maximal degree ≥ 6 .

Mathematical model from [5] is based on the fact that every polyhedron P which is composed from a single polymer chain can be naturally represented by a graph $G(P)$ of the polyhedron. Since in the self-assembly process every edge of $G(P)$ corresponds to a coiled-coil dimer, exactly two segments are associated with every edge of $G(P)$. Polyhedral graph P is then realized by interlocking pairs of polypeptide chains if its corresponding graph $G(P)$ contains a closed walk which traverses every edge exactly twice (double trace). For polyhedral nanostructure to be stable and not fall apart or self-assemble into a structure of different shape than desired, additional conditions are required, therefore strong traces are being used. The two coiled-coil-forming segments can either be aligned in the same direction or in the opposite direction, which can be simulated with parallel or antiparallel edges in double trace, respectively.

Further usage of novel self-assembly strategy in [13] also mark re-blossoming of protein origami, which has spent the better part of the past decade overshadowed by DNA origami. Since the diversity of coiled-coil-forming segments is limited, protein origami also exposes the problem of selecting an optimal set of segments in polypeptide chain to maximize the probability that self-assembled polyhedron will be stable. In this direction we define E -restricted strong traces and use them as an upgrade of current mathematical model which gives fuller control over the process of self-assembling and makes predicting the properties of outcome structure easier and more accurate.

In present paper we characterize graphs which admit E -restricted strong and d -stable traces (with respect to given set E).

Unless said otherwise, all graphs considered in this paper will be connected, finite, and simple (without any loops and parallel edges). We denote the degree of a vertex v by $d_G(v)$ or $d(v)$ for short if graph G is clear from the context. The *minimum degree* of G is denoted with $\delta(G)$, while $\Delta(G)$ is used for *maximal degree* of G . If v is a vertex then $N(v)$ denotes a set of vertices adjacent to v , and $E(v)$ is the set of edges incident with v . Graph in which all vertices are of even degree is called *even graph*. Analogously, graph with all vertices of odd degree is an *odd graph*. Note, to not confuse this with a

term *even component* (or *odd component*) which we use for a connected component of graph that has an even (or odd) number of edges. A term *Eulerian graph* is also used for even connected graph, since such graph admits Eulerian circuit. A *spanning tree* T in G is a connected subgraph of G which includes every vertex of G and is without any cycle. By removing edges of T from G we construct a *co-tree* $G - E(T)$ which is not necessary connected.

Let $E' \subseteq E(G)$. We denote a multigraph that we get from a simple graph G by replacing every connected component of a subgraph $G_{E'}$ induced by edges from E' with a single vertex, while maintaining all the edges from $E(G) \setminus E'$, with G/E' . Those new vertices in G/E' are then called E' -vertices. We also call every vertex contained in a subgraph $G_{E'}$ E' -vertex.

For any other terms and concepts from graph theory and topological graph theory not defined here we refer to [22] and [14], respectively.

2 Double traces and E -restrictions

A *walk* in G is an alternating sequence

$$W = w_0 e_1 w_1 \dots w_{\ell-1} e_{\ell} w_{\ell}, \quad (1)$$

so that for each $i = 1, \dots, \ell$, e_i is an edge between vertices w_{i-1} and w_i . We say that W *passes through* or *traverses* edges and vertices contained in the sequence (1). The *length* of a walk is the number of edges in the sequence, and we call w_0 and w_{ℓ} the *endvertices* of W . A walk is *closed* if its endvertices coincide.

Closed walk which traverses every edge of a graph exactly twice is called *double trace*. Using fundamental Euler's theorem it was observed by many authors that every connected graph admits a double trace. Let W be a double trace of length ℓ in graph G , v a vertex in G and $N \subseteq N(v)$ a subset of its neighbors. We say that W admits an *N -repetition* at v if whenever W visits v coming from a vertex in N it also returns to a vertex of N . An example of a repetition can be seen on Fig. 1. More formally W has a N repetition if the following implication holds:

$$\text{for every } i \in \{0, \dots, \ell - 1\}: \text{ if } v = w_i \text{ then } w_{i+1} \in N \text{ if and only if } w_{i-1} \in N. \quad (2)$$

Note that we treat a double trace as a closed walk taking indices in (2) modulo ℓ . This implies that w_1 is the vertex immediately following w_{ℓ} . An N -repetition (at v) is a *d -repetition* if $|N| = d$, and a d -repetition will also be called a *repetition of order d* . An N -repetition at v is *trivial* if $N = \emptyset$ or $N = N(v)$. Clearly if W has an N -repetition at v , then it also has an $N(v) \setminus N$ -repetition at v . In [5] a *d -stable trace* was defined as a double trace without any nontrivial repetition of order $\leq d$ and a *strong trace* was defined as a double trace without any nontrivial repetitions. Note that the term strong trace was in some other papers used to describe (antiparallel) 1-stable traces, which will not be the case in present paper. It was also observed in [5] that if $\delta(G) > d$ then

every strong trace in G is also a d -stable trace. If in addition $\Delta(G) < 2d + 2$ is true, then also every d -stable trace is strong trace.

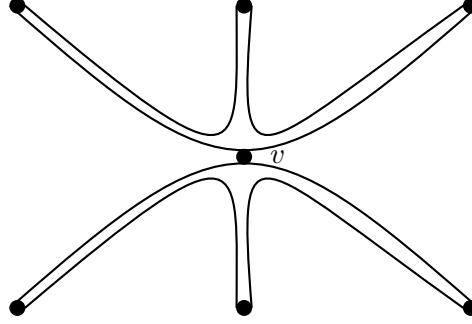


Figure 1: 3-repetition at vertex v of degree 6

Since every edge $e = uv$ is traversed exactly twice in a double trace W , we consider two cases. If e is traversed twice in the same direction (either both times from u to v or both times from v to u) then we call e a *parallel edge* (with respect to W), otherwise e is an *antiparallel edge*. A double trace W is a *parallel double trace* if every edge of G is parallel and an *antiparallel double trace* if every edge of G is antiparallel.

Graphs admitting different strong and d -stable traces were characterized in [5, 16] (previously 1-stable and 2-stable traces where under different names also investigated in [4, 12, 15, 17, 18, 19]), where next results were proven using a connection between strong traces and single face embeddings of graphs.

Theorem 2.1 [5, Theorem 2.4] *Every connected graph G admits a strong trace.*

Proposition 2.2 [5, Proposition 3.4] *Let G be a connected graph. Then G admits a d -stable trace if and only if $\delta(G) > d$.*

Theorem 2.3 [5, Theorem 4.1] *A graph G admits an antiparallel strong trace if and only if there exists a spanning tree T of G with the property that every connected component of co-tree $G - E(T)$ has an even number of edges.*

Theorem 2.4 [16, Theorem 2.5] *Let $d \geq 1$ be an integer. A graph G admits an antiparallel d -stable trace if and only if $\delta(G) > d$ and there exists a spanning tree T of G with the property that every component of co-tree $G - E(T)$ is even or contains a vertex v , $d_G(v) \geq 2d + 2$.*

Theorem 2.5 [5, Theorem 5.3] *Graph G admits a parallel strong trace if and only if G is Eulerian.*

Theorem 2.6 [5, Theorem 5.4] *Let $d \geq 1$ be an integer. A connected graph G admits a parallel d -stable trace if and only if G is Eulerian and $\delta(G) > d$.*

Note also that if G_M is a multigraph (loops and parallel edges allowed), W a double trace of G_M and v its vertex we can for $N \subseteq E(v)$ analogously as for simple graphs define an N -repetition of W at v and consequently also define strong and d -stable traces. Following two lemmas then readily follows from the fact that if v is a vertex of graph (or multigraph) G of degree 2 and W is a strong trace of G , then after we reach v on W from u , the trace W continues to the unique neighbor of v different from u .

Lemma 2.7 *Let G_M be a multigraph and G a simple graph constructed from G_M by replacing every loop and parallel edge with disjunctive path of length 3 and 2, respectively. G_M admits a strong trace if and only if G admits a strong trace. Furthermore, if both G_M and G have strong traces, then for every strong trace W in G exist a strong traces W_M in G_M which traverses common edges in the same direction as W and loops and parallel edges in the same direction as paths replacing them.*

Lemma 2.8 *Let G_M be a multigraph and G a simple graph constructed from G_M by replacing every loop and parallel edge with disjunctive path of length 3 and 2, respectively. Let $V \subseteq V(G_M)$. G_M admits a double trace with nontrivial repetitions appearing only in vertices from V if and only if G admits a double trace with nontrivial repetitions appearing only in vertices from V . Furthermore, if both G_M and G have a double trace with nontrivial repetitions appearing only in vertices from V , then for every such double trace W in G exist a double traces W_M in G_M which traverses common edges in the same direction as W and loops and parallel edges in the same direction as paths replacing them.*

We now make the key definition of this paper:

Definition 2.9 *Let G be a connected graph and $E \subseteq E(G)$. A double trace W in G where every edge from E is antiparallel and every edge from $E(G) \setminus E$ is parallel is called a E -restricted double trace.*

Analogously we, for a graph G and $E \subseteq E(G)$, define an E -restricted strong trace and an E -restricted d -stable trace as a strong trace and a d -stable trace in which every edge from E is antiparallel and every edge from $E(G) \setminus E$ is parallel, respectively.

Interestingly, E -restricted double traces first appeared almost fifty years ago, when Wagner [21] posed (in our language) a problem to characterize graphs, which admits E -restricted double traces. The problem was later independently solved by Vastergaard in [20] and by Fleischner [8] as follows:

Theorem 2.10 [20, Theorem 2], [8, Theorem VIII.13.] *Let G be a connected graph and $E \subseteq E(G)$. G admits an E -restricted double trace if and only if $G - E$ is an even graph.*

More about double traces in general can be found in [7, 8].

3 Graphs that admit E -restricted strong traces and Xuong trees approximations

The main result of this paper can be read as follows:

Theorem 3.1 *Let G be a connected graph, $E \subseteq E(G)$, and $E' = E(G) \setminus E$. Graph G admits an E -restricted strong trace if and only if:*

- *a subgraph G'_E induced by E' is an even subgraph,*
- *there exists a spanning tree T of G/E' with the property that every connected component of $G/E' - E(T)$ has an even number of edges or contains an E' -vertex.*

Theorem 2.1 implies that (at least in theory) every connected graph G can be constructed from a single chain containing coiled-coil-forming segments. Since the number of coiled-coil-forming segments simultaneously interlocking into a nanostructure is limited, Theorem 3.1 explains in details, the arrangement of those segments in a chain for a desire structure to be designed via self-assembling.

Before presenting the proof of Theorem 3.1 in Section 4, we prove a few lemmas later used in the proof of Theorem 3.1 in the rest of this section.

Lemma 3.2 *Let G be a graph and W_1 and W_2 two distinct closed walks in G . Let there exists a vertex v contained in both W_1 and W_2 . Then W_1 and W_2 can be merged into a single closed walk W which traverses every edge from W_1 and W_2 in G .*

Proof. Denote vertex preceding and following v in W_1 with u_1 u_2 , respectively, and vertices preceding and following v in W_2 with u_3 u_4 , respectively. Let edges connecting them to v be e_1, e_2, e_3 , and e_4 , respectively. Let us start walking along W_1 . When we come to v from u_1 on e_1 , we continue along e_4 to u_4 and follow W_2 . When we come back to v from u_3 on e_3 , continue on e_2 to u_2 and we continue along W_1 . This implies that the walks W_1 and W_2 merge into a single closed walk, see Fig. 2.

□

Next observation was to some extend already presented in [5].

Lemma 3.3 *Let G be a graph, W a double trace of G and v a vertex in G such that W has at least two nontrivial repetitions R_1 and R_2 in v . Let W uses edge $e = uv \in R_1$ twice in the same direction. There exists an alternative double trace W' which preserve the orientation of edges being traversed in W and has strictly fewer nontrivial repetitions in v (and in general).*

Proof. Choose an edge $e = uv \in R_1$ so that W uses e in the direction towards v twice. Let $e_2 = vu_2$ and $e_3 = vu_3$ be the edges from R_1 that immediately succeed both

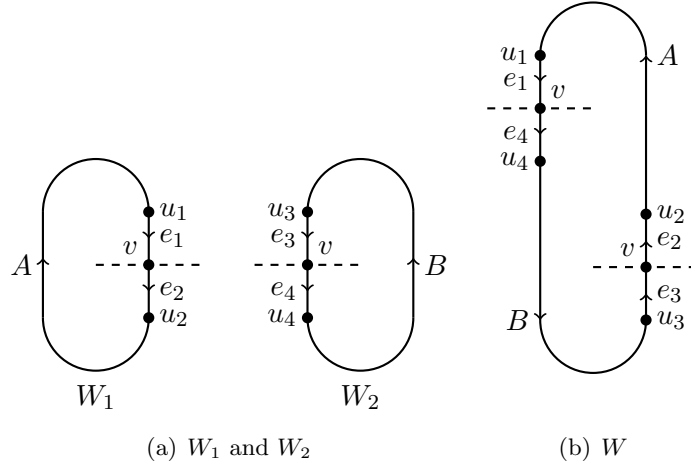


Figure 2: Construction of a single closed walk using two closed walk with common vertex

occurrences of e along W (note that e_2 may be equal to e_3). Next let $e_4 = u_4v$ and $e_5 = vu_5$ be edges from R_2 so that $u_4e_4ve_5u_5$ is a subsequence of W .

Without loss of generality (by choosing an alternative initial vertex along W) we may assume that

$$W = \dots ueve_2u_2Aueve_3u_3Bu_4e_4ve_5u_5C\dots,$$

where A , B , and C are three “interior” subwalks of W between the three shown occurrences of v in W . Observe the following walk

$$W' = \dots ueve_3u_3Bu_4e_4ve_2u_2Aueve_5u_5C\dots$$

obtained by interchanging the two “interior” subwalks A and B , also see Fig. 3.

As W' traverses the same collection of edges (in the same direction) as W , the walk W' is indeed a double trace which preserve the orientation from W . If a vertex $x \neq v$ then the new collection of repetitions (trivial or nontrivial) of W' at x equals the original collection of repetitions of W at x , since every pair e, e' of edges meeting at x are consecutive along W' if and only if they are consecutive along W .

Now W' only changes pairs of consecutive edges from $R_1 \cup R_2$, hence the only possible repetitions of W' at v which are not present in a collection of repetitions of W at v consist of edges from $R_1 \cup R_2$. Now the adjacencies $e - e_2$ and $e_4 - e_5$ were replaced by $e_2 - e_4$ and $e - e_5$ which implies that R_1 and R_2 merge into exactly one repetition in a collection of repetitions of W' at v containing all edges from $R_1 \cup R_2$. Hence the total number of nontrivial repetitions has decreased by at least one (by two if $R_1 \cup R_2$ is trivial).

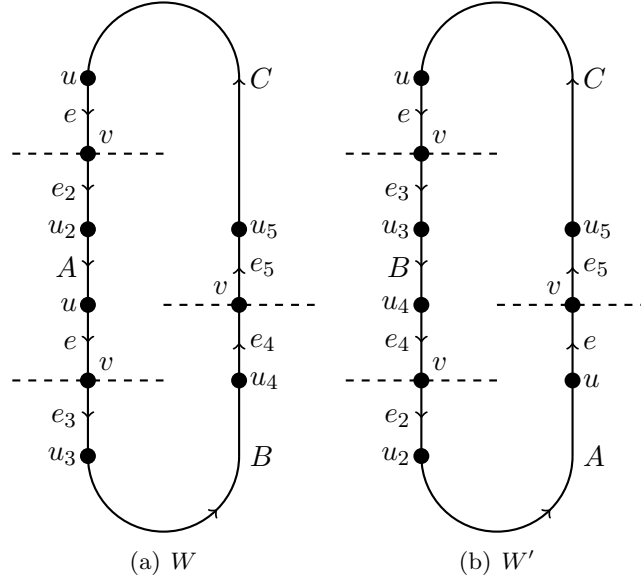


Figure 3: Decreasing the number of nontrivial repetitions in double trace

Analogously if e is used twice in direction away from v . \square

It is not difficult to find an example where W' from Lemma 3.3 does not exist if edge e is not traversed twice in the same direction in W , or if vertex v appears at most twice in W . Therefore it follows that all conditions from Lemma 3.3 are also necessary.

Next lemmas extend results about spanning trees, presented by Xuong in [23, 24], where a connection between single face embeddings of graphs into orientable surfaces and spanning trees was established. For a spanning tree T of graph G a term *deficiency* represents a number of odd connected components in a co-tree $G - E(T)$ and T is a *Xuong tree* if its deficiency is minimal among all spanning trees in G (deficiency of T is then also a *deficiency of graph G*). For the purposes of characterizing graphs admitting antiparallel d -stable traces, as seen in Theorem 2.4, we are more interested in Xuong tree approximations in which we additionally demand that every odd connected component of co-tree contains a vertex with certain properties.

Lemma 3.4 *Let G be a graph, $V \subseteq V(G)$ and T a spanning tree of G with the property that every connected component of co-tree $G - E(T)$ is even or contains a vertex from V . Denote l arbitrary vertex with disjunctive neighborhoods in G with v_1, \dots, v_l . Construct G' from G by replacing vertices v_1, \dots, v_l with new vertex v and adjacent their neighbors to it. Then there exists a spanning tree T' of G' with the property that each connected component of $G - E(T')$ is even, contains a vertex from V , or contains v .*

Proof. Construct T' from T as follows. Let $e = xy$ be an edge from T . If $x, y \notin \{v_1, \dots, v_l\}$, put e in T' . For $x \in \{v_1, \dots, v_l\}$, replace e with vy in T' . Analogously for $y \in \{v_1, \dots, v_l\}$, replace e with xv in T' . Clearly every cycle in T' contains an edge from $E(v)$. Remove them until T' is not a spanning tree of G' . Since every connected component of $G' - E(T')$ not containing v has its copy in G , it is even or contains a vertex from V . Remaining connected component contains v . \square

Repeating the construction from the proof of Lemma 3.4 at most k times, next lemma easily follows.

Lemma 3.5 *Let G be a graph, $V \subseteq V(G)$ and T a spanning tree of G with the property that every connected component of co-tree $G - E(T)$ is even or contains a vertex from V . Denote l arbitrary vertices with disjunctive neighborhoods in G with $v_{1,1}, \dots, v_{1,l_1}, \dots, v_{k,1}, \dots, v_{k,l_k}$, where $\sum_{i=1}^k l_i = l$. Construct G' from G by replacing vertices $v_{i,1}, \dots, v_{i,l_i}$ with new vertex v_i and adjacent their neighbors to it. Then there exists a spanning tree T' of G' with the property that each connected component of $G - E(T')$ is even, contains a vertex from V , or contains at least one of the newly vertices v_1, \dots, v_k .*

Since loop is never part of a spanning tree and at most one of the parallel edges is contained in a spanning tree of multigraph next lemma about spanning trees in multigraphs is also true.

Lemma 3.6 *Let G_M be a multigraph, $V \subseteq V(G_M)$ and G a simple graph obtained from G_M by replacing loops and parallel edges with disjoint paths of length 3 or 2, respectively. Assume also that for every loop or parallel edge, V contains at least one of its endvertices. If there exists a spanning tree T of G with the property that every connected component of co-tree $G - E(T)$ is even or contains a vertex from V it follows, that G_M has such a spanning tree as well.*

Note that for a spanning tree of multigraph, consequently edges incident with both endvertices of a parallel loop are always in the same connected component of its co-tree.

Next lemma explains the connection between above described approximation of Xuong trees and antiparallel double traces.

Lemma 3.7 *Let G be a connected graph and $V \subseteq V(G)$. G admits an antiparallel double trace where nontrivial repetitions appear only in vertices from V , if and only if there exists a spanning tree T of G with the property that each connected component of $G - E(T)$ is even or contains a V -vertex.*

Proof. Let W be an antiparallel double trace of G with nontrivial repetitions appearing only in vertices from $V \subseteq V(G)$. Let r be the power of V . If $r = 0$, Theorem 2.3 ensures that there exists a spanning tree T of G with the property that every connected

component of $G - E(T)$ has an even number of edges. Therefore T is a spanning tree with the property that every connected component is even or contains a vertex from V as well.

Let next $r \geq 1$ and v be one of the vertices in which W has a nontrivial repetitions (denote them with N_1, \dots, N_k). Obtain a graph G_1 from G as follows. Replace vertex v with k new nonadjacent vertices v_1, \dots, v_k in G , where k is equal to the number of repetitions of W at v . Add edges between v_i and the vertices from N_i for $1 \leq i \leq k$. The rest of the graph G is unchanged. Next construct a double trace W_1 in G_1 from W as follows. Start in an arbitrary vertex of $V(G) \cap V(G_1)$ and follow W . Let $e = xy$ be an edge of W that we are currently traversing on our walk along W . If $x, y \neq v$, then we put xy into W_1 so that the order of edges from W is preserved. Replace edges, where $x = v$ and $y \in N_i$ or $x \in N_i$ and $y = v$ with $v_i y$ or $x v_i$, for $1 \leq i \leq k$, respectively. Obviously the number of vertices with nontrivial repetitions in W_1 has decreased by exactly one comparing to W . Repeating the same procedure on all the vertices in which W has nontrivial repetitions, give us a graph G_r which admits an antiparallel strong trace and therefore (by Theorem 2.3) there exists a spanning tree T_r of G_r with the property that each connected component of $G_r - E(T_r)$ has an even number of edges. It follows from Lemma 3.5 that there exists a spanning tree T of G with the property that each connected component of $G - E(T)$ is even or contains a vertex from V .

Conversely, let G be a connected graph, $V \subseteq V(G)$, and T a spanning tree of G with the property that each connected component of $G - E(T)$ is even or contains a vertex from V . Let $\chi(T)$ represent the number of odd connected components in $G - E(T)$, and assume that T is a spanning tree with minimal $\chi(T)$ in G . If $\chi = \chi(T) = 0$, Theorem 2.3 ensures that G admits an antiparallel strong trace.

Let next $\chi = \chi(T) \geq 1$ and $v \in V$ be one of the vertices contained in one of odd connected components of $G - E(T)$. Since v is contained in an odd connected component of $G - E(T)$, we can partition $E(v)$ into two nonempty sets: E_T with edges from spanning tree T and E_C with edges from odd connected component of $E(v) \cap (G - E(T))$. Since T is a spanning tree there exists a unique path in T between an endvertex of any edge in E_T and an endvertex any edge in E_C . Construct new graph G_1 from G as follows. Replace vertex v with two new vertices v' and v'' . Replace v in edges from E_T with v' and with v'' in edges from E_C . G_1 is clearly connected graph. Since v is contained in an odd component C of $G - E(T)$, there exists an edge $e \in E_C$ such that the number of edges in a component that we get from C if we disconnect e in v is also odd (note that this can also be the whole C). Subgraph T_1 obtained from T with adding such e to it is clearly its spanning tree for which the number of odd components in $G_1 - E(T_1)$ is strictly smaller than χ , see Fig. 4 for details.

Repeating the same procedure at arbitrary vertex from V in all odd connected components of co-tree $G - E(T)$, give us a graph G_χ in which exists a spanning tree T_χ with the property that every connected component of co-tree $G_\chi - E(T_\chi)$ has an even number of edges. Therefore, by Theorem 2.3 G_χ admits an antiparallel strong trace W_χ . Let $e = xy$ be an edge in G_χ , $x \notin V(G)$ and $v \in V$ a vertex which was during the

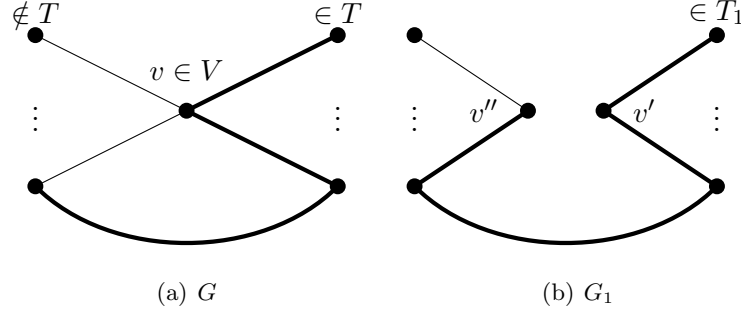


Figure 4: Construction of spanning tree T_1 in G_1 from T in G . Edges contained in spanning trees are drawn thick.

construction replaced with x . Replacing e with vy in W_χ and consecutively in the same way replacing other edges having endvertices not contained in $V(G)$ we can construct an antiparallel double trace in G for which nontrivial repetitions only appear in vertices from V . \square

4 Proof of Theorem 3.1

In this section we prove the main result of our paper — Theorem 3.1.

Proof. Let G be a connected graph, $E \subseteq E(G)$, $E' = E(G) \setminus E$, and W an E -restricted strong trace of G . Let v be an arbitrary vertex incident with an edge from E' in G . Since W traverses every edge from E' twice in the same direction, it follows that every edge from E' incident with v is used by W exactly twice for entering v or exactly twice for leaving v . Analogously, since W traverses every edge from E once in each direction, it follows that every edge from E incident with v is used by W exactly once for entering v and exactly once for leaving v . Therefore it follows, that if v is incident with an odd number of edges from E' the number of W entering v does not match the number of W leaving the v , which is absurd.

We next construct a double trace W_E in G/E' from W as follows. Start in an arbitrary vertex of $V(G/E') \cap V(G)$ and follow W . Let $e = xy$ be an edge of W that we are currently traversing on our walk along W . If $xy \in E$, then we put xy into W_E so that the order of edges from W is preserved. If x was during the construction of G/E' merged into a new vertex z , we replace xy with zy in W_E . Analogously, if y was merged into a new vertex z , xy is replaced with xz . The occurrences of edges from E' are ignored in W_E . We claim that W_E is an antiparallel double trace of G/E' . Note that any edge e' that appears in G/E' has its unique corresponding edge e in G . Since e

is traversed twice in opposite directions in W , the edge e' is traversed twice in opposite direction in W' .

Next, replace any potential loop or parallel edge in G/E' with a path of length 3 or 2, respectively, to construct a simple graph G' from G/E' . Construct an antiparallel double trace W' in G' from W_E as follows. We start in an arbitrary vertex of $V(G') \cap V(G/E')$, follow W_E and add every edge from $E(G/E') \cap E(G')$ into W' so that the order of edges from W_E is preserved. Traverses of loops and parallel edges from W_E are replaced with traverses of paths of length 3 or 2 which replaced them in W' . W' is clearly an antiparallel double trace of G' . We claim that nontrivial repetitions appear only in E' -vertices in W' . Therefore we look at three different cases. Let first v be a vertex of degree 2 which was added while replacing loops and parallel edges with paths of length 2. Denote its neighbors with u and w . Since we replaced uw (and wu) from W_E with uvw (and wvu) in W' , v is without nontrivial repetitions. In the second case let v be a vertex without any E' -vertex in its neighborhood (and also not being an E' -vertex itself). Every alternating sequence $uevfw$, where u and w are neighbors of v in G' and e and f are edges connecting them to v , appears in W' if and only if the same alternating sequence also appears in W_E (even more, it also appears in W). Therefore if W' has a nontrivial repetition at v also W would have a nontrivial repetition at v , a contradiction. Let for our final case v be a non E' -vertex in $V(G')$ and u an E' -vertex neighbor of v . We can assume that uv is not a loop or a parallel edge in G/E' since we have already taken care for such vertices in first case. During the construction of G/E' and consequently G' , u replaced a set of vertices $U \subseteq V(G)$ such that exactly one of them was adjacent to v (otherwise uv would be a parallel edge of G/E'). Denote this vertex with u_G . Therefore if W' has a nontrivial N -repetition in v such that $u \in N \subseteq N_{G'}(v)$, W has a nontrivial N -repetition in v such that $u_G \in N \subseteq N_G(v)$. It follows that W' is an antiparallel double trace of G' , where nontrivial repetitions only appear in E' -vertices.

It follows from Lemma 3.7 that there exists a spanning tree T' of G' with the property that every connected component of its co-tree $G' - E(T')$ is even or contains an E' -vertex. Therefore, by Lemma 3.6, G/E' admits such spanning tree as well.

Conversely, let G be a connected graph, $E \subseteq E(G)$ and $E' = E(G) \setminus E$. Let subgraph G'_E induced by E' be an even subgraph and let there exists a spanning tree T of G/E' with the property that every connected component of $G/E' - E(T)$ has an even number of edges or contains an E' -vertex.

Denote connected components of subgraph induced by E' with E'_1, \dots, E'_k ($k \geq 1$). Since a subgraph induced by E' is an even subgraph, also each of its component is even and therefore Theorem 2.5 implies that every E'_i admits a parallel strong trace W'_i . Lemma 3.7 also implies that G/E' admits an antiparallel double trace W' , where nontrivial repetitions appear only in E' -vertices. Note here that if $k = 0$, it follows that $E = E(G)$, G/E' is isomorphic to G , and therefore, by Theorem 2.3, G admits an antiparallel strong trace W , which is also an E -restricted strong trace for given

$E = E(G)$. Analogously, if $E = \emptyset$ it follows that $k = 1$ and by Theorem 2.5, G has a parallel strong trace W which is also an E -restricted strong trace for given $E = \emptyset$.

We first construct a set of walks \mathcal{W}_E in G which combine contain every edge from E exactly twice, once in each direction, from W' . Walks in \mathcal{W}_E will be denoted with $W_{E,i}$, where i is positive integer while for the vertices constructed from subgraph G'_E in G we will use $V' = v_1, \dots, v_k$. Let first $i = 1$. Start in an arbitrary vertex v_j , $1 \leq j \leq k$ and follow W' . Let $e = xy$ be an edge of W' that we are currently traversing on our walk along W' . We put xy into $W_{E,i}$ so that the order of edges from W is preserved. If $x \in V'$ (as is the case for the first edge) put zy into $W_{E,i}$, where zy is an edge which in G corresponds to xy in G/E' . Analogously, if $y \in V'$ put xz into $W_{E,i}$ and after that also increase i by one. We finish when we return back to initial vertex v_j and an initial edge e is the next edge to travel. We can naturally divide \mathcal{W}_E into two parts: \mathcal{W}_C and \mathcal{W}'_C , where first consists of all closed walks from \mathcal{W}_E and the other from the rest of them. The walks from \mathcal{W}'_C are of two forms — those with both endpoints contained in unique E'_i and those having one endpoint in E'_i and the other endpoint in E'_j , where $i \neq j$, respectively.

We consider those two cases to merge walks from \mathcal{W}_E and parallel strong traces W'_i , $1 \leq i \leq k$ into a set of closed walks \mathcal{W}' . Let in the first case W_C be an arbitrary walk from \mathcal{W}_C and W'_i one of the parallel strong traces which has a common vertex with W_C (at least one such parallel strong trace exists). Let v be one of the common vertices between W_C and W'_i . Place yourself in v and start walking along W_C . When returning back to v and the next edge to travel on W_C would be the same as the initial one, we continue to W'_i until traversing every edge of it exactly twice before returning back to v . This implies that the walks W_C and W'_i merge into a single closed walk. Let in the second case W_{C1} be an arbitrary walk from \mathcal{W}'_C and W'_i a parallel strong trace in which a last endpoint v of W_{C1} is contained. Denote another walk from \mathcal{W}'_C which has an initial endpoint in v with W_{C2} . Such walk clearly exists since otherwise the number of times parallel double traces W'_1, \dots, W'_k and walks from \mathcal{W}_E enters v is different than the number of times parallel double traces W'_1, \dots, W'_k and walks from \mathcal{W}_E exits v , which is absurd. We merge W_{C1} and W_{C2} into a single walk at v . Using the same argument we can in finitely many steps construct a closed walk using (not necessarily all) walks from \mathcal{W}'_C . This walk can then be, as described in previous case merged with W'_i .

We have those constructed a set of closed walks \mathcal{W}' in G which combine contain every edge from $E(G)$ twice and edges from E' are traversed twice in the same direction while edges from E are traversed once in each direction. Additionally, every closed walk from \mathcal{W} traverses at least one edge twice in the same direction. If \mathcal{W} contains more than one walk, then there exists a vertex v which is contained in at least two of them — W_1 and W_2 . Lemma 3.2 states that we can merge W_1 and W_2 into a new closed walk to produce a new set of closed walks \mathcal{W} in G which combine contain every edge from $E(G)$ twice (edges from E' being traversed twice in the same direction and edges from E being traversed once in each direction) for which $|\mathcal{W}| < |\mathcal{W}'|$. By the induction on the number of walks contained in \mathcal{W} , it follows that G has a double trace W which

traverse every edge from E' twice in the same direction and every edge from E once in each direction. We can argue that every vertex which has a repetition in W is adjacent to edges from both E and E' , since otherwise, we would have a nontrivial repetition in some of parallel strong traces W'_i or a nontrivial repetition in a non E' -vertex of antiparallel double trace W' , which is absurd.

Denote the set of vertices where W yields nontrivial repetitions with V (V is a subset E' -vertices). Let r be the power of V . If $r = 0$ then W is a strong trace and Theorem 3.1 is proven. Let next $r \geq 1$ and let v be one of the vertices where W has nontrivial repetitions. Lemma 3.3 ensures that there exists a double trace in G for which the number of nontrivial repetitions has decreased by at least one at v comparing to W , while other vertices and direction of edges remains unchanged. By two inductions, first on the number of nontrivial repetitions at v and second on the number r , it follows that G admits an E -restricted strong trace. \square

5 Generalization to d -stable traces

Since a strong trace in G is d -stable, provided that no vertex in G has degree $\leq d$ Theorem 3.1 easily implies a d -stable version of it.

Theorem 5.1 *Let G be a connected graph, d a positive integer, $E \subseteq E(G)$, and $E' = E(G) \setminus E$. Graph G admits an E -restricted d -stable trace if and only if $\delta(G) > d$ and:*

- *a subgraph G'_E induced by E' is an even subgraph,*
- *there exists a spanning tree T of G/E' with the property that every connected component of $G/E' - E(T)$ is even or contains a vertex v , $d_{G/E'}(v) \geq 2d + 2$ or contains an E' -vertex.*

6 Directed versions of Theorems 3.1 and 5.1

In this section we prove the directed versions of Theorems 3.1 and 5.1. Therefore we first recall some definitions about mixed graphs. A *mixed graph* G consisting of a set of vertices $V(G)$, a set of (undirected) edges $E(G)$, and a set of directed edges or *arcs* $A(G)$. For every subset $X \subseteq V(G)$, $e(X)$, $a^+(X)$, and $a^-(X)$ represent edges incident with X , arcs starting at X , and arcs ending in X , respectively. A mixed graph is called *weakly connected* if replacing all of its directed edges (arcs) with undirected edges produces a connected (undirected) graph.

Next theorem was independently proven by Ford and Fullkerson in [9] and later by Batagelj and Pisanski in [2] and Fleischner in [6].

Theorem 6.1 [9, Theorem 7.1] [6, Theorem IV.11.] *Let G be a weakly connected mixed graph. Then any two of the following statements are equivalent:*

1. For every $X \subseteq V(G)$, $f_G(X) = e(X) - |a^+(X) - a^-(X)|$ is a non-negative even integer.
2. G has an Euler tour W .
3. G has a cycle decomposition S .

Characterization of mixed graphs which admit E -restricted strong traces that traverse directed edges (arcs) of a graph twice in the prescribed direction then easily follows.

Theorem 6.2 *Let G be a weakly connected mixed graph, $E \subseteq E(G)$, and $E' = E(G) \setminus E$. Mixed graph G admits an E -restricted strong trace, where edges from $A = A(G)$ are traversed twice in the prescribed direction, if and only if:*

- for every vertex v in a subgraph $G_{E' \cup A} \subseteq G$ induced by $E' \cup A$, $e(v) = |a^+(v) - a^-(v)|$,
- for every connected component B of $G_{E' \cup A}$ and for every $X \subseteq V(B)$, $f_B(X)$ is a non-negative even integer,
- there exists a spanning tree T of $G/(E' \cup A)$ with the property that every connected component of $G/(E' \cup A) - E(T)$ has an even number of edges or contains an $(E' \cup A)$ -vertex.

Note that first item from Theorem 6.2 is a mixed graph analogy for an even subgraph in undirected graphs.

Proof. Theorem 6.1 implies that every connected component B in a subgraph $G_{E' \cup A}$ induced by edges from $E' \cup A$ has an Eulerian tour W' that traverses every edge from A in the prescribed direction. Therefore we can, for every component B in $G_{E' \cup A}$, construct a parallel double trace W by traversing W' twice. Since none of the operations that we are using in the proof Theorem 3.1 changes the orientation of the edges, the rest follows if we use exactly the same steps as in the proof of Theorem 3.1. \square

Analogously we can characterize graphs which admits E -restricted d -stable traces that traverse directed edges (arcs) of a graph twice in the prescribed direction.

Theorem 6.3 *Let G be a weakly connected mixed graph, d a positive integer, $E \subseteq E(G)$, and $E' = E(G) \setminus E$. Mixed graph G admits an E -restricted d -stable trace, where edges from $A = A(G)$ are traversed twice in the prescribed direction, if and only if $\delta(G) > d$ and:*

- for every vertex v in a subgraph $G_{E' \cup A} \subseteq G$ induced by $E' \cup A$, $e(v) = |a^+(v) - a^-(v)|$,

- for every connected component B of $G_{E' \cup A}$ and for every $X \subseteq V(B)$, $f_B(X)$ is a non-negative even integer,
- there exists a spanning tree T of $G/(E' \cup A)$ with the property that every connected component of $G/(E' \cup A) - E(T)$ has an even number of edges or contains a vertex v , $d_{G/(E' \cup A)}(v) \geq 2d + 2$ or contains an $(E' \cup A)$ -vertex.

7 Conclusion

In 1998 Benevise López and Soler Fernández corrected Thomassen's proof of Theorem 3.4 from [18]. More formally, they proved that there exists a polynomial algorithm which determine if there exists a spanning tree T of graph G with the property that every connected component of its co-tree $G - E(T)$ is even or contains a vertex of degree at least 4 by using Gabow and Stallman algorithm for spanning tree parity problem from [10]. Then they described how this spanning tree can be used to find an antiparallel 1-stable trace of G in polynomial time. With small modification, the same algorithm can be used for determining if graph G admits antiparallel d -stable trace. Therefore, it follows that we can check if graph fulfills conditions from Theorems 3.1 and 5.1 and consequently has a desired double trace in polynomial time.

Let us finish with an open problem, again deriving from self-assembly polypeptide nanostructure design. Two double traces W and W' are called *equivalent* if W' can be obtained from W by reversion W , by shifting W , by applying a permutation on W induced by an automorphisms of G , or using any combination of the previous three operations. Note that equivalence classes of strong traces were defined and thoroughly investigated in [1, 12].

Problem 7.1 Find an efficient algorithm, which for a given graph G and a positive integer p , returns all non-equivalent E -restricted strong traces, where $|E| = p$.

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